Dr. rer. nat. Alexander Urban
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Experience

Since 08/2025	Associate Professor, Columbia University, New York, NY, USA
01/2019–07/2025	Assistant Professor, Columbia University, New York, NY, USA
01/2018–12/2018	Independent University Fellow, University of St Andrews, UK
09/2015–12/2017	Research Specialist, University of California, Berkeley, CA, USA
10/2012–08/2015	Postdoctoral Associate, Massachusetts Inst. of Technology, Cambridge, MA, USA

Education

10/2008–09/2012	Ph.D. (Dr. rer. nat.), Friedrich-Alexander-University Erlangen-Nuremberg, Germany
10/2006–09/2008	M.Sc., Chemistry, Ruhr-University Bochum, Germany
10/2003–09/2006	B.Sc., Chemistry, Ruhr-University Bochum, Germany

Peer-Reviewed Publications (Google Scholar: https://scholar.google.com/citations?user=swpn0HUAAAAJ)

1. B. Donovan, A. West, and **A. Urban***, r^{2}SCAN+rVV10+*U* parameterization for 3*d* transition metal sulfides for thermochemistry, *J. Chem. Phys.* **163** (2025) 034707.
2. I.-W. Yeu, A. Stuke, J. López-Zorrilla, J. M. Stevenson, D. R. Reichman, R. A. Friesner, **A. Urban***, N. Artrith*, Scalable training of neural network potentials for complex interfaces through data augmentation, *npj Comput. Mater.* **11** (2025) 156.
3. C. Komurcuoglu, A. C. West, **A. Urban***, The mechanism of the layered-to-spinel phase transformation in $Li_{0.5}NiO_2$ from first principles, *ACS Appl. Energy Mater.* **7** (2024) 10784–10794.
4. V. Gharakhanyan, L. Wirth, J. A. Garrido Torres, E. Eisenberg, T. Wang, D. R. Trinkle, S. Chatterjee, and **A. Urban***, Discovering melting-temperature prediction models of inorganic solids by combining supervised and unsupervised learning, *J. Phys. Chem.* **160** (2024) 204112.
5. C. Cao†, M. R. Carbone†, C. Komurcuoglu, J. S. Shekhawat, K. Sun, H. Guo, S. Liu, K. Chen, S.-M. Bak, Y. Du, C. Weiland, X. Tong, D. Steingart, S. Yoo, N. Artrith, **A. Urban***, D. Lu*, F. Wang*, Atomic Insights into the Oxidative Degradation Mechanisms of Sulfide Solid Electrolytes, *Cell Rep. Phys. Sci.***5** (2024) 101909.
6. **A. Urban***, Modeling ionic transport and disorder in crystalline electrodes using percolation theory, Book chapter in D. A. H. Hanaor (editor), *Computational Design of Battery Materials*, Springer 2024, ISBN: 978-3-031-47302-9; preprint: https://doi.org/10.48550/arXiv.2302.06759
7. H. Guo, M. R. Carbone, C. Cao, J. Qu, Y. Du, S.-M. Bak, C. Weiland, F. Wang, S. Yoo, N. Artrith, **A. Urban***, and D. Lu*, Simulated sulfur K-edge X-ray absorption spectroscopy database of lithium thiophosphate solid electrolytes, *Sci. Data* **10** (2023) 349.
8. Y. Xiao, P. Zheng, T. Yang, S. K. Chakravarty, J. Rodriguez-Lopez, **A. Urban**, and Z. Li, Integrated Combinatorial Synthesis, Characterization, and Test Platform for Lithium-Ion Battery Cathode Materials, *J. Electrochem. Soc.* **170** (2023) 050538.
9. V. Gharakhanyan, M. S. Aalto, A. Alsoulah, N. Artrith, and **A. Urban***, Constructing and Compressing Global Moment Descriptors from Local Atomic Environments, Peer-reviewed contribution to the *ML4Materials workshop at the ICLR 2023*, https://openreview.net/forum?id=4Hl8bjobpl9
10. A. Mishra, D. Sarbapalli, Md S. Hossain, Z. T. Gossage, Z. Li, **A. Urban**, J. Rodríguez-López, Highly Sensitive Detection and Mapping of Incipient and Steady-State Oxygen Evolution from

Operating Li-Ion Battery Cathodes via Scanning Electrochemical Microscopy, *J. Electrochem. Soc.* **169** (2022) 086501.

11. H. Guo, Q. Wang, **A. Urban***, and N. Artrith*, Artificial-Intelligence-Aided Mapping of the Structure-Composition-Conductivity Relationships of Glass-Ceramic Lithium Thiophosphate Electrolytes, *Chem. Mater.* **34** (2022) 6702–6712.
12. X. Li, Q. Wang, H. Guo, N. Artrith, and **A. Urban***, Understanding the onset of surface degradation in $LiNiO_2$ cathodes, *ACS Appl. Energy Mater.* **5** (2022) 5730–5741.
13. X. Li, X. Li, L. Monluc, B. Chen, M. Tang, P.-H. Chien, X. Feng, I. Hung, Z. Gan, **A. Urban***, and Y.-Y. Hu*, Stacking-Fault Enhanced Oxygen Redox in Li_2MnO_3, *Adv. Energy Mater.* **12** (2022) 2200427.
14. N. Artrith, J. A. Garrido Torres, **A. Urban**, and M. S. Hybertsen, Data-driven Approach to Parameterize SCAN+U for an Accurate Description of 3d Transition Metal Oxide Thermochemistry, *Phys. Rev. Mater.* **6** (2022) 035003.
15. J.A. Garrido Torres, V. Gharakhanyan, N. Artrith, T.H. Eegholm, **A. Urban***, Augmenting zero-Kelvin quantum mechanics with machine learning for the prediction of chemical reactions at high temperatures, *Nat. Commun.* **12** (2021) 1-9.
16. Z. Cai, H. Ji, Y. Ha, J. Liu, D.-H. Kwon, Y. Zhang, **A. Urban**, E.E. Foley, R. Giovine, H. Kim, Z. Lun, T.-Y. Huang, G. Zeng, Y. Chen, J. Wang, B.D. McCloskey, M. Balasubramanian, R.J. Clément, W. Yang, G. Ceder, Realizing continuous cation order-to-disorder tuning in a class of high-energy spinel-type Li-ion cathodes, *Matter* **4** (2021) 3897-3916.
17. H. Guo, Q. Wang, A. Stuke, **A. Urban**, N. Artrith, Accelerated Atomistic Modeling of Solid-State Battery Materials With Machine Learning, *Frontiers Energy Res.* **9** (2021) 265.
18. A.M. Miksch, T. Morawietz, J. Kästner, **A. Urban**, N. Artrith, Strategies for the Construction of Machine-Learning Potentials for Accurate and Efficient Atomic-Scale Simulations, *Mach. Learn.: Sci. Technol.* **2** (2021) 031001.
19. Q. Wang, L. Wu, **A. Urban**, H. Cao, P. Lu, Anisotropic to Isotropic Transition in Monolayer Group-IV Tellurides, *Materials* **14** (2021) 4495.
20. J. Qu and **A. Urban***, Potential and pH dependence of the buried interface of membrane-coated electrocatalysts, *ACS Appl. Mater. Interfaces* **12** (2020) 52125-52135.
21. Z. Jadidi, T. Chen, P. Xiao, **A. Urban**, and G. Ceder, Effect of fluorination and Li-excess on the Li migration barrier in Mn-based cathode materials J, *Mater. Chem. A* **8** (2020) 19965-19974.
22. A. Cooper, J. Kästner, **A. Urban**, and N. Artrith, Efficient Training of Accurate Neural Network Potentials Including Atomic Force Information: Application to Water and Transition-Metal Oxide, *npj Comput. Mater.* **6** (2020) 54.
23. M. A. Cambaz, **A. Urban**, S. A. Pervez, H. Geßwein, A. Schiele, A. A. Guda, A. Bugaev, A. Mazilkin, T. Diemant, R. J. Behm, T. Brezesinski, M. Fichtner, Understanding the origins of higher capacity for Ni-based cation-disordered rocksalt cathodes, *Chem. Mater.* **32** (2020) 3447-3461.
24. H. Ji, J. Wu, Z. Cai, J. Liu, D.-H. Kwon, H. Kim, **A. Urban**, J. K. Papp, E. Foley, Y. Tian, M. Balasubramanian, H. Kim, R. J. Clement, B. D. McCloskey, W. Yang, and Gerbrand Ceder, Ultrahigh power and energy density in partially ordered lithium-ion cathode materials, *Nat. Energy.* **5** (2020) 213–221.
25. B. Ouyang, N. Artrith, Z. Lun, Z. Jadidi, D. A. Kitchaev, H. Ji, **A. Urban**, and G. Ceder, Effect of Fluorination on Lithium Transport and Short-Range Order in Disordered-Rocksalt-Type Lithium-Ion Battery Cathodes, *Adv. Energy Mater.* **10** (2020) 1903240.
26. H. Ji, **A. Urban**, D. A. Kitchaev, D.-H. Kwon, N. Artrith, C. Ophus, W. Huang, Z. Cai, T. Shi, J. C. Kim, and G. Ceder, Hidden structural order controls Li-ion transport in cation-disordered oxides for rechargeable lithium batteries, *Nat. Commun.* **10** (2019) 592.
27. H. Kim, D.-H. Seo, **A. Urban**, J. Lee, D.-H. Kwon, S.-H. Bo, T. Shi, J. K. Papp, B. D. McCloskey, and G. Ceder, Stoichiometric Layered Potassium Transition Metal Oxide for Rechargeable Potassium Batteries, *Chem. Mater.* **30** (2018) 6532-6539.

28. N. Artrith, **A. Urban**, and G. Ceder, Constructing first-principles phase diagrams of amorphous LixSi using machine-learning-assisted sampling with an evolutionary algorithm, *J. Chem. Phys.* **148** (2018) 241711 (Editor's Pick).
29. **A. Urban***, A. Abdellahi, S. Dacek, N. Artrith, and G. Ceder*, The electronic-structure origin of cation disorder in transition-metal oxides, *Phys. Rev. Lett.* **119** (2017) 176402 (featured on phys.org).
30. H. Das, **A. Urban**, W. Huang, and G. Ceder, First-principles simulation of the (Li-Ni-Vacancy)O phase diagram and its relevance for the surface phases in Ni-rich Li-ion cathode materials, *Chem. Mater.* **29** (2017) 7840–7851.
31. G. S. Gautam, P. Canepa, **A. Urban**, S.-H. Bo, and G. Ceder, Influence of inversion on Mg mobility and electrochemistry in spinels, *Chem. Mater.* **29** (2017) 7918–7930.
32. N. Artrith, **A. Urban**, and G. Ceder, Efficient and accurate machine-learning interpolation of atomic energies in compositions with many species, *Phys. Rev. B* **96** (2017) 014112.
33. W. Huang, **A. Urban**, Z. Rong, Z. Ding, C. Luo, and G. Ceder, Construction of ground-state preserving sparse lattice models for predictive materials simulations, *npj Comput. Mater.* **3** (2017) 30.
34. W. Huang, D. Kitchaev, S. Dacek, Z. Rong, **A. Urban**, S. Cao, C. Luo, and G. Ceder, Finding and proving the exact ground state of a generalized Ising model by convex optimization and MAX-SAT, *Phys. Rev. B* **94** (2016) 134424 (Editor's Suggestion).
35. A. Abdellahi, **A. Urban**, S. Dacek, and G. Ceder, Understanding the effect of cation disorder on the voltage profile of lithium transition-metal oxides, *Chem. Mater.* **28** (2016) 5373–5383.
36. **A. Urban**, I. Matts, A. Abdellahi, and G. Ceder, Computational design and preparation of cation-disordered oxides for high-energy-density Li-ion batteries, *Adv. Energy Mater.* **6** (2016) 1600488; Highlighted with frontispiece.
37. D.-H. Seo, J. Lee, **A. Urban**, R. Malik, S. Y. Kang, and G. Ceder, The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials, *Nat. Chem.* **8** (2016) 692–697.
38. A. Abdellahi, **A. Urban**, S. Dacek, and G. Ceder, The effect of cation disorder on the average Li intercalation voltage of transition metal oxides, *Chem. Mater.* **28** (2016) 3659–3665.
39. **A. Urban**, D.-H. Seo, and G. Ceder, Computational understanding of Li-ion batteries, *npj Comput. Mater.* **2** (2016) 16002 (Review).
40. N. Artrith* and **A. Urban***, An implementation of artificial neural-network potentials for atomistic materials simulations: Performance for TiO_2, *Comp. Mater. Sci.* **114** (2016) 135–150 (Editor's Choice).
41. D.-H. Seo, **A. Urban**, and G. Ceder, Calibrating transition-metal energy levels and oxygen bands in first-principles calculations: Accurate prediction of redox potentials and charge transfer in lithium transition-metal oxides, *Phys. Rev. B* **92** (2015) 115118.
42. R. Wang, X. Li, L. Liu, J. Lee, D.-H. Seo, S.-H. Bo, **A. Urban**, and G. Ceder, A disordered rock-salt Li-excess cathode material with high capacity and substantial oxygen redox activity: $Li_{1.25}Nb_{0.25}Mn_{0.5}O_2$, *Electrochem. Commun.* **60** (2015) 70–73.
43. G. S. Gautam, P. Canepa, A. Abdellahi, **A. Urban**, R. Malik, and G. Ceder, The intercalation phase diagram of Mg in V_2O_5 from first-principles, *Chem. Mater.* **27** (2015) 3733–3742.
44. N. Twu, X. Li, **A. Urban**, M. Balasubramanian, J. Lee, L. Liu, G. Ceder, Designing new lithium-excess cathode materials from percolation theory: Nanohighways in $Li_xNi_{2-4x/3}Sb_{x/3}O_2$, *Nano. Lett.* **15** (2015) 596–602.
45. **A. Urban**, J. Lee, and G. Ceder, The configurational space of rocksalt-type oxides for high-capacity lithium battery electrodes, *Adv. Energy Mater.* **4** (2014) 1400478; Highlighted with frontispiece.
46. J. Lee, **A. Urban**, X. Li, D. Su, G. Hautier, and G. Ceder, Unlocking the potential of cation-disordered oxides for rechargeable lithium batteries, *Science* **343** (2014) 519–522.
47. **A. Urban**, M. Reese, M. Mrovec, C. Elsässer, and B. Meyer, Parameterization of tight-binding models from density functional theory calculations, *Phys. Rev. B* **84** (2011) 155119.
48. K. Katsiev, M. Batzill, and U. Diebold; **A. Urban**, and B. Meyer, Growth of one-dimensional Pd nanowires on the terraces of a reduced SnO_2(101) surface, *Phys. Rev. Lett.* **98** (2007) 186102.

49. Y. Wang, X. Xia, **A. Urban**, H. Qiu, J. Strunk, B. Meyer, M. Muhler, and Ch. Wöll, Tuning the reactivity of oxide surfaces by charge-accepting adsorbates, *Angew. Chem. Int. Ed.* **46** (2007) 7315.

Other Publications

50. N. Artrith, **A. Urban**, Y. Wang, and G. Ceder, Atomic-scale factors that control the rate capability of nanostructured amorphous Si for high-energy-density batteries, https://arxiv.org/abs/1901.09272 (2019).
51. W. Huang, **A. Urban**, P. Xiao, Z. Rong, H. Das, T. Chen, N. Artrith, A. Toumar, and G. Ceder∗, An L_0L_1-norm compressive sensing paradigm for the construction of sparse predictive lattice models using mixed integer quadratic programming, https://arxiv.org/abs/1807.10753 (2018).
52. G. Ceder, J.H. Lee, **A. Urban**, X. Li, S. Kim, G. Hautier, High-capacity positive electrode active material, US Patent 9,780,363 (2017).

Courses Taught at Columbia

1. 2019–2025, Columbia University, *Analysis of Chemical Engineering Problems* (CHEN E3020), Junior-level B.Sc. core (mandatory) course of Chemical Engineering
   This mandatory core course introduces numerical methods and computer-aided problem-solving with a specific focus on chemical engineering applications (e.g., the design of a compressor and heat exchanger). The course is graded based on reports for six applied projects and oral presentations. On average, 25-35 students.
2. 2019–2025, Columbia University, *Atomistic Simulations for Science and Engineering* (CHEN E4880), graduate-level elective course; newly developed in 2019
   This elective course targets engineering students without prior experience in atomic-scale simulations. It, therefore, not only covers atomistic simulation methods but also reviews crystallography, quantum mechanics, and statistical mechanics. The course is graded based on four project reports. On average, 40–50 students. The course has been taken by (senior) B.Sc., M.Sc., and Ph.D. students from various programs, including Chemical Engineering, Materials Science, Applied Physics and Applied Mathematics, Mechanical Engineering, and Biomedical Engineering.

Theses sponsored

- 5/6/2024, Xinhao Li; Dissertation title: Quantum-Mechanistic-Based and Data-Driven Prediction of Surface Degradation and Stacking Faults in Battery Cathode Materials
- 4/5/2024, Vahe Gharakhanyan; Dissertation title: Advancing Computational High-Temperature Materials Thermodynamics with Machine Learning
- 3/14/2024, Jianzhou Qu; Dissertation title: Towards an Atomic-scale Understanding of Membrane-coated Electrocatalysts for Hydrogen Production
- 1/26/2024, Cem Komurcuoglu; Dissertation title: Understanding Degradation Mechanisms in Cobalt-free Lithium-ion Battery Cathodes from First Principles

Select Recent Invited Talks and Seminars

2025/10, Invited speaker at the 248th ECS Meeting in Chicago, First-Principles Computational Tools for Electrochemical Metal Extraction, Title: *First-Principles Computational Tools for Electrochemical Metal Extraction*, Symposium F07 - *Atomistic Modeling of Electrochemical Systems.*

2025/08, Keynote speaker at the 28th International Annual Symposium on Computational Science and Engineering, Thammasat, Pathum Thani, Thailand.

2025/05, Invited department seminar in the Department of Radiation Science and Technology, TU Delft, The Netherlands (Host: Prof. Jan Leen Kloosterman)

2024/07, Keynote speaker at the 27th International Annual Symposium on Computational Science and Engineering, Chulalongkorn University, Bangkok, Thailand.

2023/11, Invited department seminar in the Department of Materials Science and Chemical Engineering, Stony Brook University (Host: Prof. Nav Nidhi Rajput)

2023/11, Invited department seminar in the Department of Physics, Binghamton University (Host: Prof. Alexey Kolmogorov)

2023/10, Invited department seminar in the School of Chemistry, Suranaree Institute of Technology, Thailand (Host: Prof. Suwit Suthirakun)

2023/09, Invited department seminar in the Department of Chemical Engineering, TU Delft, Netherlands (Host: Prof. Evgeny Pidko)2023/08, Invited talk in the symposium "Data-Driven Design of Energy Materials" at the ACS Fall Meeting, San Francisco

2023/03, Invited talk in the Hume-Rothery Symposium at the TMS Annual Meeting, San Diego

2022/11, Invited department seminar at Pusan National University, Busan, South Korea (Hosts: Prof. Joonyung Jang and Prof. Yongchul Chung)

2022/11, Invited talk at the 7th International Conference on Electronic Materials and Nanotechnology for Green Environment, Jeju, South Korea.

2021/09, Invited department seminar at NJIT, Newark, NJ (Host: Prof. G. Gor).

2021/07, Invited (virtual) NY-BEST lecture on degradation in lithium-ion batteries.

2021/06, Invited (virtual) department seminar at the Fritz-Haber Institute, Berlin, Germany (Hosts: Dr. J. Margraf and Prof. K. Reuter).

2020/11, Invited (virtual) department seminar in the Institute for Energy and Climate Research, Jülich Research Centre, Germany (Host: Dr. P. Kowalski and Prof. M. Eikerling)

2020/02, Invited seminar in the Department of Chemical Engineering & Materials Science at Stevens Institute of Technology, Hoboken, NJ (Host: Prof. J.-C. Kim)

Awards

- 2024 NSF CAREER Award
- In 2019, Named *Scialog Fellow* for *Advanced Energy Storage* by the Research Corporation for Science Advancement
- Kekulé Fellowship of the *Fonds der Chemischen Industrie*, Germany (2008–2011)
- Wilke Prize (year's top Master's graduate), *Verein zur Förderung der Chemie und Biochemie*, Ruhr–University Bochum, Germany, in 2008

Recent Synergistic Activities

- Chair of the 2024 & 2021 *AIChE Battery and Energy Storage Conference* in New York City; Organizing board member in 2020, 2022, and 2023
- Since 2024, member of the *Columbia Empire AI Working Group*
- Since 2023, chair of the *Shared Research Computing Policy Advisory Committee (SRCPAC)* for high-performance computing at Columbia University
- Founding and core faculty member of the *Columbia Center for Computational Electrochemistry* (CCCE), a collaboration with *Schrödinger Inc.*
- Founding and core faculty member of the *Columbia Electrochemical Energy Center (CEEC)*
- Member of the editorial board of *IOP Model. Simul. Mater. Sci. Eng.*
- Chair of the section 1E session "Lithium and Beyond" at the 2022 annual AIChE meeting in Phoenix, AZ; Co-chair of the section 1E session "Lithium and Beyond" at the 2021 annual AIChE meeting in Boston, MA
- Co-organizer of the tutorial workshop *Machine-Learning for Materials Science* held in parallel with the Machine Learning in Science & Engineering 2020 conference.

Outreach Activities

- Organizer, Mini-ASESMA summer school at the University of Ibadan, Nigeria, August 5-9, 2024.
- Lecturer at the 7th *African School on Electronic Structure Methods and Applications* - ASESMA 2023 (https://indico.ictp.it/event/10181), Kigali, Rwanda, June 12–23, 2023
- In the summers of 2022 and 2023, contributed projects at The Coding School (TCS) by codeConnects (https://codeconnects.org) that offers summer courses in data science for high-school students.
- With support from the U.S.-Africa Initiative in Electronic Structure, hosted Dr. Olugbenga Oshakuade (University of Ibadan, Nigeria) and Dr. Catherine Paschal (Mwenge Catholic University, Tanzania), during summer 2022. This visit started an ongoing collaboration with Dr. Oshakuade.
- Guest speaker at the Spellman HV Clean-Tech Competition 2019, an international research and design challenge for high-school students from all over the world
- 2018 Interview with Seeker Media (Discovery Communications) on lithium-ion batteries for non-experts: https://youtu.be/ZnWW0P-7paE (>170,000 views).